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VALIDITY AND ACCURACY OF ATMOSPHERIC AIR QUALITY MODELS

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1. INTRODUCTION

Effective evaluation of air pollution control strategies requires the use of validated and reliable mathematical models that can relate pollutant emissions to atmospheric air quality. The derivation and use of such models, at least for inert and linearly decaying pollutants such as CO and SO_2, has received a great deal of attention. Much less work has been devoted to assessing how the model predictions are related to actual atmospheric concentrations. The objectives of this paper are to formulate the concepts of validity and accuracy and to suggest and describe some experiments that can be performed to assess these features.

2. VALIDITY OF THE ATMOSPHERIC DIFFUSION EQUATION

Validity in the context of this paper is defined as a measure of how well the mathematical model describes the physics and chemistry of the atmosphere. Discrepancies in validity arise as a consequence of the need to employ physical assumptions in the formulation of the model. Assumptions may be required either because of ignorance of the physical processes or of the need for economy in the final numerical solution. More formally, validity can be defined as how closely the exact solution of the model equations corresponds to the true atmospheric concentrations.

At present, routine solutions are not available to the coupled mass, momentum, energy and state equations which describe, on an urban scale, the dynamics of the atmosphere. As a result, most conventional atmospheric diffusion models are based on a simplified approach that uses only the species conservation equation (1).

$$\frac{\partial c_i}{\partial t} + \underset{\sim}{u} \cdot \nabla c_i = D_i \nabla^2 c_i + R_i(c_1,\ldots,c_N,T)+S_i \qquad (1)$$

Where c_i is the concentration of species i, $\underset{\sim}{u}$ is the carrier fluid velocity with components [u,v,w] in the three co-ordinate directions, D_i is the molecular diffusivity of species i in the air, R_i is the generation of species i due to chemical reaction at temperature T among the N species and S_i the rate of injection of species i into the fluid from source emissions. A major practical difficulty with the solution of (1) is that the fluid dynamic fields in turbulent flows are always unsteady and depend strongly on the finest details of the initial conditions, details of which are never available with sufficient precision. A consequence of the turbulent flow is that the velocity and concentration fields are both random functions of space and time.

By decomposing the fluid velocities into a mean and fluctuating part, $u = \bar{u} + u'$, etc., where $\bar{u}$, $\bar{v}$, $\bar{w}$ represent ensemble means, and applying a similar idea to the concentration field, an expression for the ensemble mean $\bar{c}_i$ can be derived in the form (2).

$$\frac{\partial \bar{c}_i}{\partial t} + \underset{\sim}{\bar{u}} \cdot \nabla \bar{c}_i = \nabla \cdot (D_i \bar{c}_i - \overline{\underset{\sim}{u}' c_i'}) + \overline{R_i(c_1,\ldots,c_N,T)} + \bar{S}_i \qquad (2)$$

Equation (2) is rigorously valid for $\bar{c}_i$. If the variables $\overline{u'c_i'}$,... as well as those arising from R_i are known functions of space and time, (2) can, in principle, be solved to yield $\bar{c}_i$.

The appearance of the terms, $\overline{u'c'}$, $\overline{v'c'}$, $\overline{w'c'}$ leads to the classical closure problem of turbulence. In order to solve this problem approximations are made; and they represent the first source of invalidity for (2). In K - theory, the simplest closure approximation employed in many models of atmospheric diffusion, the eddy fluxes are assumed to be proportional to the negative gradient of the concentration field and are of the form

$$\overline{u'c_i'} = -K_{xx} \frac{\partial \bar{c}_i}{\partial x} \qquad \overline{v'c_i'} = -K_{yy} \frac{\partial \bar{c}_i}{\partial y}$$

$$\overline{w'c_i'} = -K_{zz} \frac{\partial \bar{c}_i}{\partial y} \qquad (3)$$

Higher order closure models will offer some improvement over eddy diffusivities but at present they are computationally expensive for routine use. (Lewellen and Teske, 1975).

While there has been considerable study of the methods for modeling terms of the form $\overline{u'c_i'}$, there has been relatively little examination of the approximation needed to solve (2) when chemical reactions take place. For example, if species i decays by a second order reaction, $I + I \xrightarrow{k}$, then the mean rate of disappearance of $\bar{c}_i$ is given by $R_i = k\bar{c}_i - \overline{kc_i'^2}$

3. ACCURACY OF THE ATMOSPHERIC DIFFUSION EQUATION

Accuracy refers to the extent of agreement between the mean concentrations predicted by (5) in practice and those predicted by (5) if the true values of all input parameters in (5) were used. For example, errors that will reduce accuracy can be introduced as a result of the fact that $\bar{u}$, $\bar{v}$, and $\bar{w}$ used in the solution of (5) are not the actual mean velocities.

3.1 ANALYSIS OF THE ACCURACY OF MODEL PARAMETERS

An analysis of the effects of approximations and uncertainty in model parameters and/or boundary conditions can be generally performed in two ways. Deterministic methods rely on sensitivity and perturbation analysis of the model predictions with respect to small changes in the parameters. These methods can determine which model variables most influence the predictions

At present, most models for chemically reactive pollutants employ the approximation that the mean rate of reaction can be approximated by the rate based on the mean concentrations,

$$\overline{R_i\ (c_1,\ldots,c_N,T)} \doteq R_i\ (\bar{c}_1,\ldots,\bar{c}_N,\bar{T}) \qquad (4)$$

This approximation has been evaluated and a new closure model developed by Lamb and Shu (1976) and Shu, et al. (1976).

The result of using (3) and (4) in (2) and neglecting molecular diffusion is the so-called atmospheric diffusion equation (ADE) upon which most current urban air pollution models for chemically reacting air pollutants are based. (See, for example, Reynolds, et al., (1973); MacCracken, et al., (1975)).

$$\frac{\partial \bar{c}_i}{\partial t} + \underset{\sim}{u}\cdot\nabla\bar{c}_i = \nabla\cdot K\nabla\bar{c}_i + R_i(\bar{c}_1,\ldots,\bar{c}_N,\bar{T}) + \bar{S}_i \qquad (5)$$

The validity of (5) refers to how closely the predicted mean concentration $\bar{c}_i$ corresponds to the true ensemble mean. Unfortunately, the atmosphere presents only one realization of the flow at any time, and unless stationarity conditions hold, unambiguous measures of the validity of (5) in any particular flow cannot be obtained. Assessment of the validity of the ADE is an extremely complex task because of the enormous practical difficulties of obtaining measurements in actual flows. With the advent of numerical turbulence simulations, assessments are becoming feasible and will be important areas for future investigation. Theoretical forms for eddy diffusivities can be examined by comparing results predicted by the ADE with those with the numerical field. (Lamb, et al., 1975). Table 1 summarizes sources of invalidity in the ADE.

Table 1. Errors in the Atmospheric Diffusion Equation (ADE)

Source of error	Comment
The true form of the turbulent fluxes, $\overline{u'c_i'}$, $\overline{v'c_i'}$, and $\overline{w'c_i'}$ are unknown.	The major source of invalidity of the ADE. Higher order closure models will offer improvement over eddy diffusivities in representing these terms.
The chemical reaction mechanism R_i does not accurately reflect the actual chemistry.	A source of invalidity for chemically reacting species. Continued study of laboratory chemistry and its relation to the atmosphere needed to minimize this source of error.
Turbulent fluctuating chemical reaction terms are neglected.	A secondary source of invalidity of the ADE. Appropriate closure models must be developed.

Table 2 summarizes the major sources of inaccuracy in applications involving the use of (5).

Table 2. Sources of Inaccuracy in the Atmospheric Diffusion Equation

Source of error	Comment
The mean velocities $\bar{u}$, $\bar{v}$, $\bar{w}$ used in the solution of the ADE are not the true ensemble means (usually u, v, and w are constructed from data at a finite number of locations).	There is no way to determine the true mean from data. $\bar{u}$, $\bar{v}$, and $\bar{w}$ can be calculated from an accurate fluid mechanical turbulence model. A source of inaccuracy of the ADE.
The source emission function S_i is inaccurate.	A source of inaccuracy. Better compilation of emission factors needed.
The ADE must be solved on a grid size consistent with the spatial detail in the wind and source emission functions.	A source of inaccuracy. Better resolution of wind and source emission fields will allow use of a finer grid.

Table 3 illustrates the inputs needed to solve the ADE; and, in each instance, unless the actual value of the input is known, the level of error can only be estimated. From the standpoint of the effects of errors on the predictions of the ADE, joint considerations must be given to the level of uncertainty and the sensitivity of the predicted concentrations to the parameter. The distinction between uncertainty and sensitivity of a parameter has important implications for the resources allocated to data collection. For example, a parameter that has a large uncertainty but has little influence in the ADE solution may not require extensive evaluation.

Table 3. Summary of Inputs Needed to Solve the Atmospheric Diffusion Equation

Input	Level of Detail	Sources of Error
Wind velocities	Variation of $\bar{u},\bar{v},\bar{w}$ with x,y,z, and t.	Measurements available only at a few locations, generally at ground level, at discrete times. Error in: 1. Variation of $\bar{u}$ and $\bar{v}$ horizontally. 2. Variation of $\bar{u}$ and $\bar{v}$ vertically. 3. Determination of $\bar{w}$.
Eddy diffusivities	Variation of K_H and K_V with z and t.	No direct measurements available. K_H and K_V must be inferred from theories. Both magnitude and vertical variation unknown.
Chemical reaction mechanism	Rate equation for each $\bar{c}_i$.	Inaccurate rates because of: 1. Inability to simulate atmosphere in the laboratory. 2. Unknown reactions. 3. Unknown rate constants.
Source emissions	Emission rate as a function of x,y,z, and t.	Inaccurate knowledge of: 1. Level of source activity. 2. Emission factors.
Boundary conditions	Location of vertical boundary as a function of x,y, and t.	Lack of data or adequate model of temperature structure of atmosphere.

3. ACCURACY OF THE ATMOSPHERIC DIFFUSION EQUATION

Accuracy refers to the extent of agreement between the mean concentrations predicted by (5) in practice and those predicted by (5) if the true values of all input parameters in (5) were used. For example, errors that will reduce accuracy can be introduced as a result of the fact that $\bar{u}$, $\bar{v}$, and $\bar{w}$ used in the solution of (5) are not the actual mean velocities.

3.1 ANALYSIS OF THE ACCURACY OF MODEL PARAMETERS

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and consequently the level of accuracy required for the input parameters. Statistical methods are based on determining the statistical properties of the model predictions with respect to the statistical properties of the input variables. Because of the complexity of (5), sensitivity and perturbation analyses are generally the methods used in evaluating uncertainty and sensitivity.

3.2 NUMERICAL ACCURACY PROBLEMS

A major area of inaccuracy that must be considered is the numerical approximations required to solve the mathematical model. Complex numerical schemes are required to solve the three-dimensional, coupled, non-linear, stiff, parabolic partial differential equations that may result from the atmospheric diffusion equation. The choice of numerical methods to be used in the approximated model are important factors that influence the accuracy and economy of the solution. In most cases, spatial and temporal discretization introduces additional averaging and a loss of characterization of subgrid scale processes. This problem can be corrected, to some extent, by the use of subgrid scale models, but they must be augmented by careful analyses of the influence of grid size and time step on the accuracy of the results.

A common source of inaccuracy in the solution of (5) is numerical truncation errors in the approximation of the advection terms. These should be minimized using, for example, high order schemes such as the zero average phase error technique of Fromm (1968) or the sign preserving SHASTA method of Boris and Book (1973). The requirements for high order accuracy must be balanced with computer resource requirements.

The accuracy of numerical schemes can, in principle, be evaluated by performing numerical experiments with problems of known analytic solutions. Tests can be used to assess the effects of numerical diffusion and the influence of dispersion on phase errors. Numerical dissipation dominates in first order difference schemes and tends to reduce the amplitude of concentration peaks, while in second-order approximations, dispersion at high wave numbers becomes the most serious problem. Dispersion is common to all methods but dissipation is absent from time-centered schemes. A common test is the Crowley (1968) "color" problem in which a conical distribution of a scalar quantity, s, is advected by a circular wind field (6).

$$\frac{\partial s}{\partial t} + \underset{\sim}{u} \cdot \nabla s = 0 \qquad (6)$$

Where $u = -(y-y_o)/16$, $v = (x-x_o)/16$, and x_o, y_o is the center of a 32 x 32 grid. This test is severe but representative of steep concentration gradients which can occur in practice. Figure 1(a),(b) illustrates the distribution of s after one complete rotation of the wind field. Figure 1(a) is the flux correcting transport (FCT) scheme of Boris and Book (1973) and 1(b) Fromm's (1968) zero average phase error (ZAPE) technique. The FCT scheme preserves the sign of positive quantities, and the height of the unit cone after one revolution is 0.51. The Fromm scheme does not preserve sign because small dispersive waves of amplitude 0.03 trail the main cone. Diffusion has reduced the cone height to 0.55. Other schemes tested showed pronounced dissipation and large phase errors.

Special consideration must be given to the character of the chemical terms and their numerical properties. Solution of the stiff system of ordinary differential equations that often arises, requires the use of Newton iteration or variable order methods like DIFSUB (Gear, 1971). Stability requirements must be carefully evaluated giving attention to the disparity of the temporal scales of the processes being modeled.

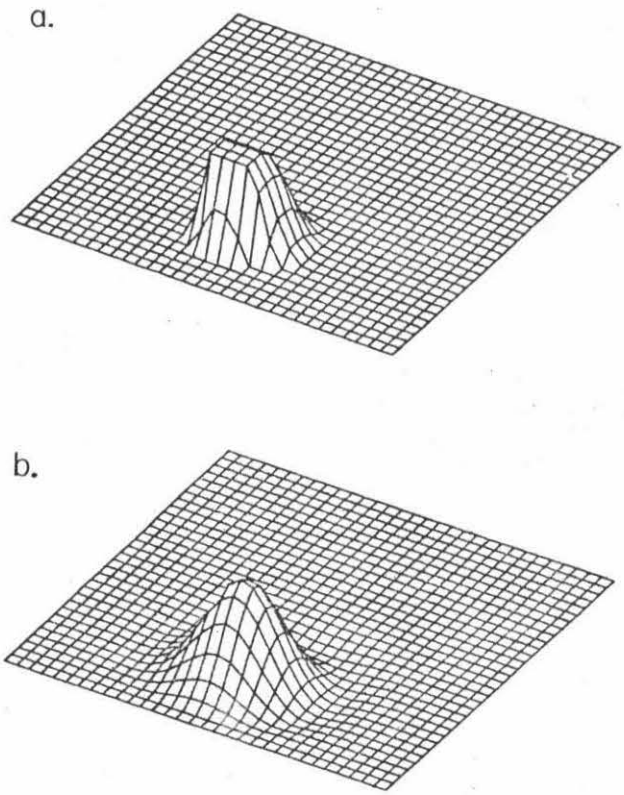

Figure 1. Results of Crowley "color" experiment for a. FCT method; and b. Fromm's ZAPE.

3.3 CHEMICAL REACTION MECHANISM

Demerjian (1975) has reviewed the sources of errors in generalized kinetic mechanisms for photochemical smog. A combined uncertainty and sensitivity study of the Hecht et al. (1974) mechanism has been carried on by Dodge and Hecht (1975). In that study it was found that several reactions were not needed and could be neglected, but they also found that 12 rate constants should be more accurately determined. It is important to note that the

above study was not concerned with the validity of the mechanism but only with the uncertainty of the rate constants and the sensitivity of the resulting species concentrations to those rate constants.

3.4 METEOROLOGICAL INPUTS

The specification of the wind fields and the vertical boundary of the model are important factors which influence the accuracy of the model predictions. There is a crucial need for objective analysis procedures which can be used on a routine basis to specify meteorological inputs to the ADE models. Generation of mass consistent wind fields from sparse and inadequate measurement data is a difficult problem. Until complete planetary boundary layer models can be developed and validated, air pollution modeling must continue to rely on the use of wind fields derived using interpolation and smoothing procedures that satisfy the dynamic constraints.

3.5 SOURCE EMISSIONS

Source emissions may be characterized according to:

1. Level of spatial resolution.
2. Level of temporal resolution.
3. Uncertainty in emission quantity:
   a. Uncertainty in source activity.
   b. Uncertainty in emission factor.

The level of spatial resolution achievable is generally as fine as one desires since the locations of all resources can presumably be specified. (Although traffic count data may not be available on a street-by-street basis). Temporal emission rates will fluctuate from day to day. For motor vehicles it is safe to employ single temporal distributions for surface streets and freeways derived from the analysis of appropriate data. The major problem in properly specifying source emissions is uncertainty in emission quantities arising from uncertainties in source activities and emission factors.

Typical levels of uncertainties in mobile and fixed source activities (e.g. number of vehicle miles travelled and number of units of fuel consumed) should be identified. Then, the typical uncertainties in emission factors (e.g., g/mi of pollutant emitted per vehicle mile travelled and g of pollutant per unit of fuel consumed) should be combined with the uncertainties in activities to produce net uncertainties in emissions. Finally, sensitivity studies should be carried out with urban diffusion models to assess the effect of these levels of uncertainties in source emissions on predicted concentrations.

3.6 INITIAL AND BOUNDARY CONDITIONS

Many of the problems with the specification of model parameters can be illustrated, in some detail, by the establishment of initial and boundary conditions. The ADE requires both initial and boundary conditions to complete the description of the system. A value for each pollutant species must be specified at each grid point initially and along the lateral boundaries at each time step.

When considering initial and boundary values it is necessary to determine:

1. What conditions are required?
2. How should these boundary and initial conditions be established and treated numerically?
3. What is the influence of inevitable uncertainties in the boundary and initial data of the model results?

The measured concentration data from which initial concentrations are to be specified

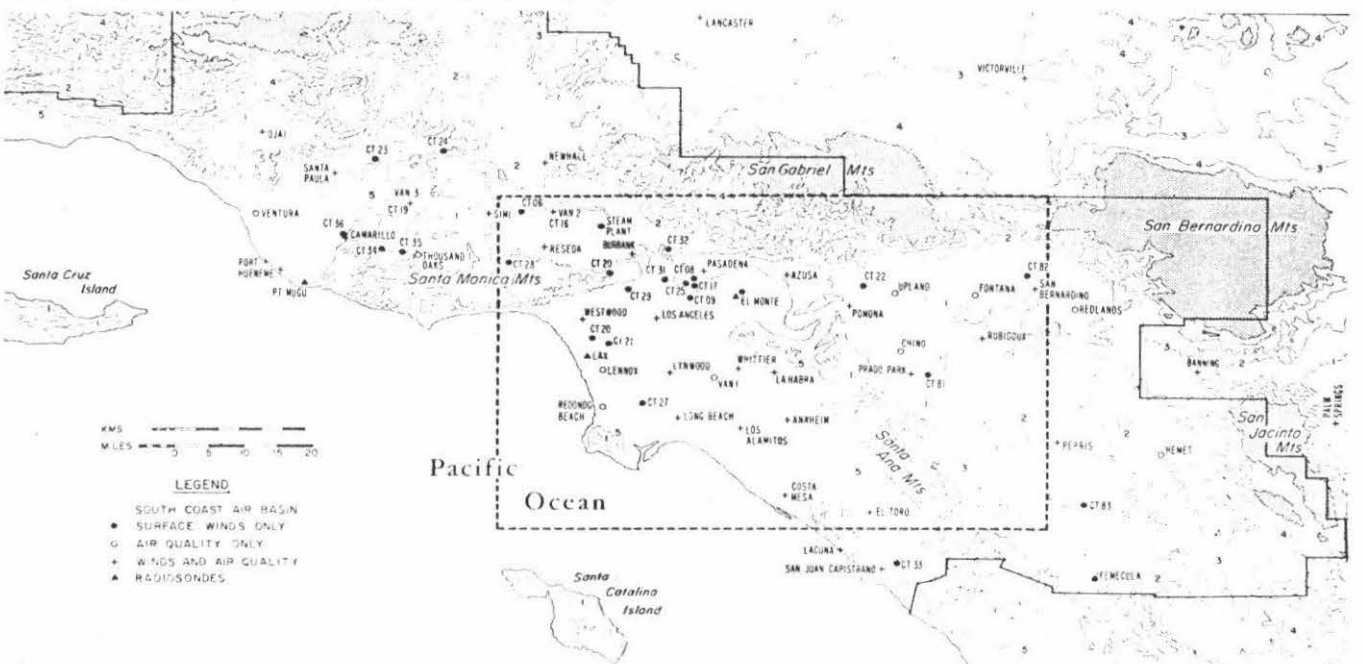

Figure 2. Map of South Coast Air Basin and surrounding area. SCAB is enclosed by solid line. Area studied by Goodin (1975) is enclosed by dotted line.

are usually sparse, irregularly spaced, and generally limited to surface stations. For example, the South Coast Air Basin, which covers approximately 15,000 square miles, has between twenty and forty measuring stations (depending on the pollutant). Therefore, in order to obtain a representative concentration field, at least at the surface, for a given hour one must interpolate the station values to grid locations.

The South Coast Air Basin can be overlayed by a 100 x 50 grid of 2 x 2 mile squares (Fig. 2). Since computer storage requirements limit the size of arrays which can be considered, we intend to solve the equations over one or more subsets of the 100 x 50 grid. Thus, if at each hour an interpolation is performed to obtain values at each grid point, initial and boundary conditions can be extracted for any desired subgrid.

Before proceeding with an analysis of interpolation procedures, the importance of the initial concentration field must be investigated. Do the initial concentrations become irrelevant after a certain number of hours? A study of this problem was made using the vertically integrated CO model of Goodin (1975). The area considered was a 40 x 25 square subset of the 100 x 50 grid (Fig. 2). The model was run for 36 hours with initial concentrations computed using a simple distance weighted interpolation scheme. The same solution procedure was then performed with zero initial concentrations. The results are displayed in Fig. 3. At each station the time history beginning at zero is always lower than that beginning at the more realistic initial value. However, at nearly all stations, the two solutions parallel each other after about six hours. LENX and LONB are slight exceptions, since each station is within two miles of the ocean where the concentration remains zero throughout the simulation due to the lack of sources. One would expect the concentrations at these stations to remain low.

One can conclude on the basis of these results that after about six hours the initial concentrations are no longer important in determining CO concentrations. The initial concentration for a photochemical pollutant may have a different relaxation time since the pollutant is non-conservative. The relaxation time may also be a function of time of day due to the influence of solar radiation.

Since the initial concentrations are relatively important, at least for CO, some care must be taken in producing a concentration surface from measured data. There are a number of techniques for interpolating irregularly spaced data to grid locations. The concentration value at a grid point can be determined from a weighted function of the values at nearby stations.

$$C_{ij} = \Sigma W_k(r)\ \hat{C}_{ij} / \Sigma W_k(r)$$

The weighting function, $W_k(r)$, may, for example, take the form $1/r^n$ or $(R^2 - r^2)/(R^2 + r^2)$, where r is the distance between the grid point and the k-th station and R is a radius of influence within which stations are used in the calculation. Alternatively, one can fit a polynomial surface to the data points in a least squares sense or fit the data using splines. Due to limited space, only the results of weighting procedures will be presented here; investigations of surface fitting is in progress.

A test case was designed to study the relative merits of three weighting factors: $1/r$, $1/r^2$, $(R^2 - r^2)/(R^2 + r^2)$. A hemispherically shaped surface centered at (50,25) was placed over the 100 x 50 grid. The height of the surface was computed at each of 34 oxidant measuring stations distributed across the basin (Fig. 4). Each of the three weighting procedures was then used to compute the values at all 5000 grid points from the 34 values. A radius of influence of 40 grid squares was used.

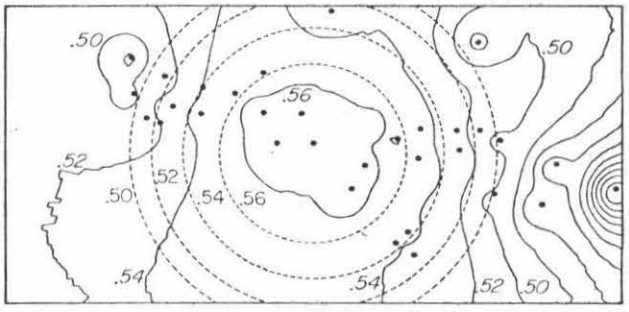

Figure 4. Results of interpolation of hemispherical data (dotted lines) using $1/r^2$ weighting procedure (solid lines). Hemisphere height is 0.58 at center of grid and 0.16 at corners (not all dotted contours are shown).

None of the three techniques was able to reproduce completely the hemispherical surface from which the 34 sampled values were taken. However, where the data were relatively closely spaced, the $1/r^2$ weighting performed best. None of the three techniques performed well in areas of sparse data. Fig. 5 shows a three-dimensional plot of the residual, $R = (Z_c - Z_t)/Z_t$ where Z_c is the computed surface height resulting from the $1/r^2$ weighting and Z_t is the theoretical surface height. The largest errors are in the areas of little data, i.e. the regions near the boundary. This is due in part to the interpolation procedure as well as the surface being tested. The large flat area in the central portion of the grid indicates small errors. Table 4 presents a summary of the percent error at the grid point for the three techniques.

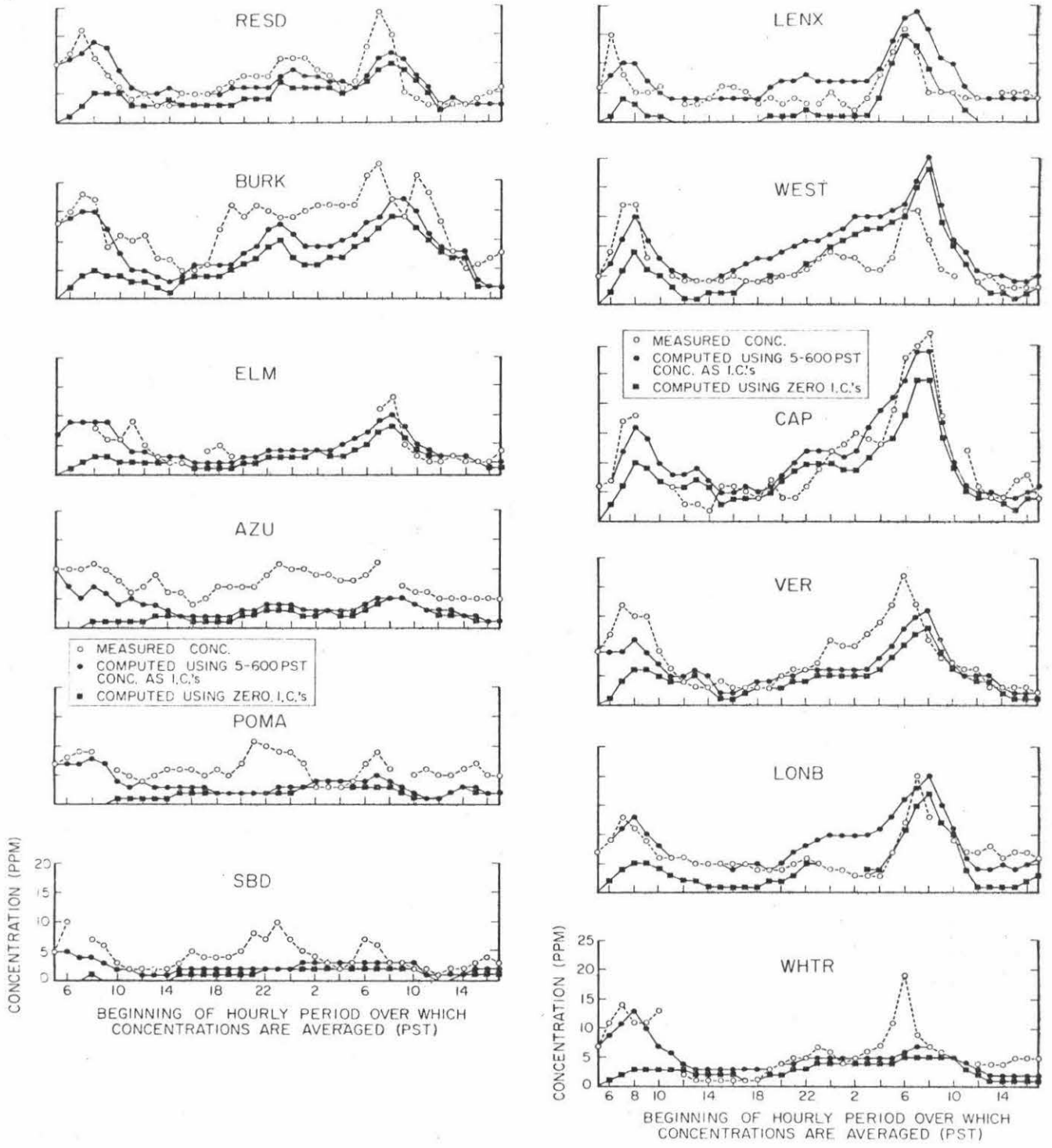

Figure 3. Time histories of concentration for 29-30 September 1969 computed using vertically integrated CO model. Results are for two runs with different initial conditions. Measurement stations can be located on Figure 2 using the following key: LENX = Lennox, WEST = West Los Angeles, VER - not shown, LONB = Long Beach, WHTR = Whittier, RESD = Reseda, BURK = Burbank, ELM = El Monte, AZU = Azusa, POMA = Pomona, SBD = San Bernardino, CAP = Los Angeles.

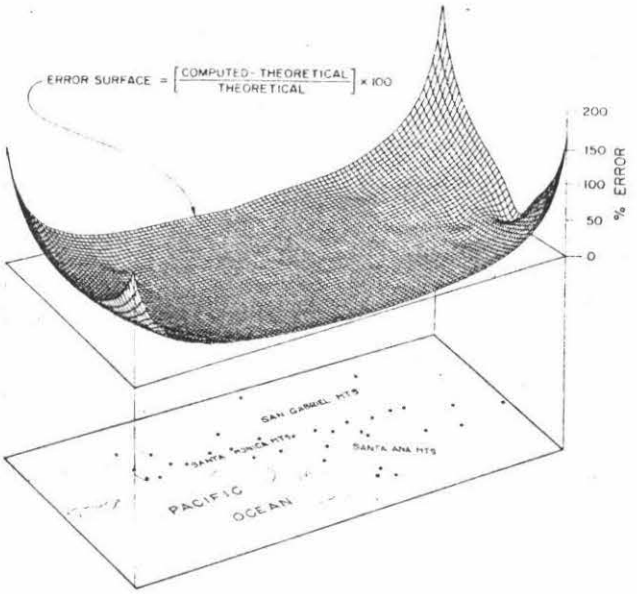

Figure 5. Three-dimensional plot of residual surface resulting from $1/r^2$ weighting procedure.

Since the polynomial and spline surface fitting procedures have not yet been examined, final conclusions cannot be drawn concerning the best scheme for producing a concentration surface from measured data. However, on the basis of the three schemes tested above, the $1/r^2$ weighting procedure yields the best fit to the idealized test data.

Table 4. Residual Error as a Function of Weighting Scheme (All values are percentages)

Weighting Scheme	Measuring Stations Only				All Grid Points			
	MEAN	MIN	MAX	S.D.	MEAN	MIN	MAX	S.D.
$1/r$	0.3	-2.2	10.1	2.4	15.4	-5.0	206.6	24.5
$1/r^2$	0.0	-0.1	0.4	0.1	13.8	-2.7	204.7	23.1
$\frac{R^2 - r^2}{R^2 + r^2}$	2.8	-8.1	64.9	13.1	16.9	-8.1	208.7	26.2

4. VALIDATION

A major practical consideration when evaluating the model and its performance is the quality of the experimental and observational results. Systematic errors are deterministic by definition and in principle can be eliminated or compensated for if they are known. They may be constant, or a function of one or more of the system parameters. Constant errors manifest themselves as a bias in the data and are undetectable except by independent measurements and physical system considerations. If the errors are not constant, they may be detected by testing the data for correlation with suspected variables or parameters. Some examples of systematic errors that can arise in air pollution and meteorological measurements are:

1. Incorrect calibration.
2. Construction defects or siting problems.
3. Inadequate regard to constancy of experimental or test conditions.
4. Failure to make necessary corrections.

Random variations are of greatest concern in the statistical analysis of measurements and can be decomposed into two types, errors due to randomness in the process, and variation due to random errors. Meteorological variables such as wind velocity, temperature, and pressure all fluctuate with time and space.

5. CONCLUSION

An understanding of the concepts of validity and accuracy is required for interpretation and proper qualification of the results of an atmospheric diffusion model. In this paper, we have suggested a number of numerical experiments that can be carried out to test the accuracy and validity of a model. Table 5 summarizes these results.

Table 5. Numerical Experiments Required to Test the Validity and Accuracy of Air Pollution Diffusion Models

Numerical Experiment	Comments
Perform diffusion experiment in numerical turbulence field and compare data with conventional air pollution models using eddy diffusivities.	Lamb et al. (1975) Lamb (1975)
Perform diffusion experiment for reactive species in numerical turbulence fields and compare data with conventional air pollution models with various reactive closure models.	
Perform sensitivity analysis of model to variations in meteorological parameters.	Liu and Whitney (1975)
Perform sensitivity analysis of model to variations in initial, boundary, and source concentrations.	Demerjian (1975)

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